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Effect of wall stiffness, mass and potential interaction strength on heat transfer characteristics of nanoscale-confined gas

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ABSTRACT

The interactive thermal wall model is applied in three-dimensional molecular dynamics simulations to investigate the combined effect of the wall force field, the wall stiffness, the wall atom mass and the wall/gas interaction potential strength on the heat transfer characteristics of static rarefied argon gas within a nanochannel. By increasing the wall stiffness, a reduction in the heat flux through the gas medium occurs which leads to a higher temperature jump. As the wall atom mass is increased up to twice the argon atom mass, the heat flux is enhanced notably and a minimum temperature jump can be found at this point. Further increase in the wall atom mass results in reducing the heat flux and consequently increasing the temperature jump. The increment of the wall/gas interaction potential strength up to four times the one of gas/gas interactions is shown to enhance the heat flux and to reduce the temperature jump until it eventually vanishes. Furthermore, it is found that under such conditions, the density profile experiences a second peak. A further increase of this parameter is found to have a negligible effect on the heat flux through the gas medium and it only increases the second peak in the density profile.

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1. Introduction

The design and performance optimization for recycling heat [1,2], efficiently using energy in buildings [3] and energy-saving applications such as thermal computers [4–6] demands a profound understanding of heat transport through gases in rarefied conditions at the nanoscale. Considering the Knudsen number $Kn = \lambda/H$ as the ratio of the gas mean free path λ to the characteristic length-scale of the domain H , complete equilibrium is achieved as $Kn \rightarrow 0$, which can be treated by the use of Euler equations. As the Knudsen number is increased, nonequilibrium effects become dominant. In the continuum regime, $Kn \leq 0.01$, where the transport is based on diffusion, the Navier-Stokes equation and the Fourier law are used to describe the momentum and heat transfer through the gas medium, respectively. In contrast, in free flight regime $Kn \geq 10$ where the transport is ballistic, the solution of the collisionless Boltzmann equation properly describes the gas characteristics.

In between these two limiting conditions, the transport can be split into two parts. For $0.01 \leq Kn \leq 1$ which is called the transition regime, a fluid description is still possible by using the Navier-Stokes equation and the Fourier law along with appropriate slip boundary conditions or higher order equations such as the Burnett equations which are the second order approximation of the Chapman-Enskog expansion for the Boltzmann equation. In the kinetic regime $1 \leq Kn \leq 10$, particle-based computer simulations such as Direct Simulation Monte Carlo (DSMC) or Molecular Dynamics (MD) method are a possible choice to approximate solutions of the Boltzmann equation. Even though they are able to properly take into account nonequilibrium contributions, due to a large number of gas atoms and molecules in this regime, they become increasingly expensive, [7–9].

The MD method was developed in the 1970s [10–12] and has advanced from simulations of several hundreds of atoms and molecules to biological systems with millions or even billions of atoms on state of the art supercomputers [13–15]. Although the best reproduction of the actual systems is obtained from atomistic simulations, coarse-grained MD is becoming very popular for long simulations or large systems [16,17]. In the MD simulation, forces acting on each atom are obtained from the force field, in which the potential energy is deduced from the molecular structure [18–20].

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The choice of the best suitable force field or the generation of new force fields for highly specific applications is still one of the major challenges in MD simulations [21–23]. Atomistic MD simulations generally require very small time steps in the region of femtoseconds which is a major bottleneck since it results in very long simulation times. Coarse-grained MD is a way to alleviate this problem by combining several atoms into a single coarse-grained particle, which allows to reduce the total number of particles in the simulation and to extend the time step by compromising on the resolved details [24–26].

In a nanoconfined medium, further complications arise due to the presence of the wall force field and the surface adsorption which requires a molecular-level resolution. The MD simulation of rarefied gas requires that the domain extends about the mean free path in the periodic directions which results in an enormous computational time. In order to reduce the computational time, Smart Wall Molecular Dynamics (SWMD) [27] and Virtual Wall Models (VWM) [28] have been proposed and the distribution of the hydrodynamic gas properties such as the gas density, velocity, pressure, and stress have been studied precisely for different Knudsen numbers [28–32]. Due to the cold wall nature of these methods, the above-mentioned simulations were limited to hydrodynamic properties and no heat transfer in the gas medium could be tackled [28,33]. A comprehensive literature review reveals that while the studies of heat transfer in a nanoconfined rarefied gas medium are restricted by the channel length in the periodic direction resulting enormous computational time, heat transfer in the nanoconfined liquid medium has been extensively studied considering appropriate wall/fluid interactions [34–45].

Heat transfer characteristics of argon gas confined in 5.4 nm channel height have been studied thoroughly [46] by implementing the interactive thermal wall model [47]. The modified Knudsen number, $k = (\sqrt{\pi}/2)Kn$, was considered as 10 which corresponds to the onset of the free molecular regime. The temperature difference between the channel walls has been varied from 10 to 200 K and the gas density, temperature and thermal resistance distributions along the channel height have been discussed comprehensively. It was shown that the combination of the implemented temperature difference and the wall force field determines the distribution of the gas atoms along the channel height. This leads to the fact that by changing the temperature differences between the walls, different normalized temperature profiles were obtained in the gas medium along the channel height. Besides, the variation of the corresponding effective thermal conductivity for each case reveals that for calculating the effective thermal conductivity based on this nonequilibrium method, the implemented temperature differences between the channel walls should not exceed 50 K [46].

Besides, the effects of two different mechanisms for changing the modified Knudsen numbers, i.e., changing the gas density at constant channel height and changing the channel height at constant gas density, on the heat transfer characteristics of the nanoconfined gas medium were studied. A wide range of the modified Knudsen numbers in the transition regime, $k = 0.1$ to 10, were considered for both mechanisms in this study. It is shown that regardless of the gas density and the channel height, approximately 1 nm from each wall is affected from the wall force field which leads to different characteristics of the gas medium in this region. In addition, it is observed that even for a channel height of 540 nm, interfacial and wall force field thermal resistance form a considerable portion of the total thermal resistance which implies the necessity of using MD simulations in even near micrometer-sized channels [48]. Recently, we have studied the effect of the implemented temperature differences on the heat transfer characteristics of nanoconfined argon gas. It was depicted

that the distribution of the gas atoms along the channel height is a function of both the temperature differences between the channel walls and the absolute temperature of each wall. Besides, the distribution of the effective local thermal conductivity and temperature profile reveals that while the diffusive transport regime exists for the dense gas, the ballistic transport regime governs the bulk region and diffusive transport is observed in the near wall region of the rarefied gas [49].

It should be considered that throughout these work, it was assumed that $m_{\text{wall}} = m_{\text{Ar}}$, $\sigma_{\text{wall}} = \sigma_{\text{Ar}}$ and $\varepsilon_{\text{wall-Ar}} = \varepsilon_{\text{Ar-Ar}}$ in order to find the general trends of the nanoconfined gas medium under heat conduction where m , σ , and ε are denoted as atom mass, atom diameter and the depth of the potential well, respectively. Furthermore, $K_S = 500\varepsilon\sigma^{-2}$ was considered as the walls spring constant in the interactive thermal wall model. A literature review reveals that the variation of these parameters can considerably affect the fluid/solid interaction which may result in a distinct momentum and heat transfer near the walls. The effects of the mass of the wall molecules and the wall stiffness on the thermal resistance at the solid/liquid interface of nanofluidic channels were investigated by the molecular dynamics method. It was shown that increasing the atomic mass of the solid molecules significantly increases the temperature jump at the interface. In addition, this effect becomes more important for the lower value of the bonding stiffness [50]. The effect of a geometrically rough wall, combined with the wettability and stiffness on the diffusion characteristics of nanoconfined liquid argon was studied by nonequilibrium molecular dynamics. It was shown that while the diffusion coefficient values are affected by the rough wall characteristics, wall wettability is the property that affects diffusion the most [51]. Furthermore, it was shown that a critical dimension exists below which all fluid properties (maximum velocity, density, temperature, slip length, shear viscosity, diffusion coefficient, and thermal conductivity) deviate from their bulk values. This critical dimension is further affected by the nanochannel wall properties [52]. The parameters affecting the slip length at the nanoscale was also investigated for liquid argon. Larger slip lengths were observed at smaller channel sizes, denser liquids, larger magnitude of the external driving forces, and higher temperatures. It was also shown that the effect of the geometric wall roughness and wall wettability on the slip length are considerable [53] and might lead to an apparent slip [54–56]. It can be observed that these studies are concentrated on liquid/solid interactions.

The objective of the current paper is to investigate the effect of wall/gas atom mass, wall stiffness and wall/gas interaction strength on the nanoconfined gas medium. We consider $0.5 \leq m_{\text{wall}}/m_{\text{Ar}} \leq 6$, $1 \leq \varepsilon_{\text{wall-Ar}}/\varepsilon_{\text{Ar-Ar}} \leq 6$ and $100\varepsilon\sigma^{-2} < K_S < 1000\varepsilon\sigma^{-2}$ for the distribution of the argon gas density, temperature, heat flux and effective thermal conductivity along a 5.4 nm channel height for $k = 1$ and 10. The above-mentioned range of selected values is consistent with typical magnitudes employed in previous MD studies [31,50,57–62] and corresponds to a broad range of real materials that are mainly used for microfluidic/nanofluidic fabrications [61,63]. Since for this channel height the wall force field covers approximately 40% of the channel height, the interaction of the wall force field and above-mentioned parameters play the main role in the distribution of different gas properties along the channel height which is discussed in detail in this manuscript.

The variation of the modified Knudsen number is achieved by changing the gas density and it is defined based on the gas density in the middle of the channel consistent with previous studies [31,48]. The exact number of argon gas atoms to produce the desired density in the center of the channel is achieved by a trial and error method as discussed below. In order to create a heat flux

through the gas medium, we assign 308K to the top wall and 288K to the bottom wall in all cases. Therefore, the mean temperature of the gas medium is defined as $T_{mean} = (308K + 288K)/2 = 298K$ and a constant temperature difference of 20K induces heat flux through the gas medium in all sets of simulations. Therefore, we can have the distribution of the thermally transport gas properties in the room temperature, i.e. 298K.

2. Simulation setup

Fig. 1 provides a schematic sketch of the perspective and the side views of the simulation domain for $k = 10$. We simulate heat conduction through the argon gas medium confined between two parallel walls that are 5.4nm apart using the MD package LAMMPS [64]. The interactive wall model is implemented on the hot (upper) and cold (bottom) walls and the remaining four boundaries are periodic. Two layers of FCC (face-centered cubic) structured atoms are used to construct the walls. The truncated (6–12) Lennard–Jones (L–J) potential,

$$V(r) = 4\epsilon \left[\left(\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right) - \left(\left(\frac{\sigma}{r_c} \right)^{12} - \left(\frac{\sigma}{r_c} \right)^6 \right) \right], \quad (1)$$

describes the van der Waals interactions between different particles, where r_c is the cutoff distance, r_{ij} is the interatomic distance between particles i and j , and $V(r_c)$ is the value of the interatomic potential at $r = r_c$. Considering the fact that the effect of the L–J potential becomes negligibly small at large molecular distance, the cut-off radius is commonly set to $r_c = 1.08nm$ for a dilute gas [30]. For the argon gas atoms, $\sigma = 0.3405nm$, $m = 6.63 \times 10^{-26}kg$ and $\epsilon = 119.8 \times K_B$ are considered, while the Boltzmann constant is $k_B = 1.3806 \times 10^{-23}J/K$. Considering this potential, the equation of motion for the particle i is given by

$$m\ddot{r} = - \sum_{i \neq j} \nabla V_{ij}^T. \quad (2)$$

We apply a velocity Verlet algorithm to integrate Newton's second law [65]. The wall particles are fixed onto their initial lattice sites by spring potentials urging them to return to their equilibrium positions r_0 via a restoring force given by

$$F_S = -K_S(r_i - r_0). \quad (3)$$

The wall stiffness (K_S) determines the strength of the bonds between the wall particles, as well as their motion. The wall atoms can exchange momentum and energy with the fluid particles. In

each layer of wall atoms, a velocity-scaling thermostat is applied in order to obtain a uniform temperature distribution in the walls. In this way, the heat is properly transferred to/from the gas through the walls and there is no need to apply any thermostat on the gas anymore [47,66]. Different temperatures for walls lead to a thermal gradient in the perpendicular direction and consequently, this gradient generates a heat flux between the parallel walls. The heat flux vector is determined by using the Irving–Kirkwood (I–K) expression [43,67],

$$J = \sum_i v_i E_i + \frac{1}{2} \sum_i \sum_{j \neq i} r_{ij} (F_{ij} \cdot v_i) - \sum_i v_i h \quad (4)$$

where E is the sum of kinetic and potential energy of the atom i , v_i is the velocity of atom i , F_{ij} denotes the two-body forces between i and j , and h is the microscopic enthalpy.

Considering the mean temperature of the gas medium as 298K, a Maxwell–Boltzmann velocity distribution is used to initialize the argon gas and wall atoms at the beginning of the simulation. Using a timestep of 4fs, we let the initial particle distribution evolve for 2×10^6 time steps (8ns) by applying a temperature-rescaling thermostat and the NVE ensemble to the wall and gas atoms. After accomplishing the thermal equilibrium, the temperature of the walls is changed to 308K and 288K allowing the system to relax towards the expected temperature difference in n_{ssc} time steps. Finally, n_{ave} timesteps are performed to average microscopic quantities in order to obtain macroscopic properties of the gas medium. In all cases, sufficiently long time averaging is also performed to confirm the convergence of macroscopic quantities such as the temperature and density profiles.

The channel height is determined from the centerlines of the first layer of wall atoms facing the gas atoms at the bottom and top surfaces. The computational domain is divided into bins of approximately 0.108nm for the density and temperature in the perpendicular direction to the walls. To improve the quality of our data, every measurement is obtained from averaging over three independent simulations. The simulation domain has the dimension of $54 \times 5.4 \times 54nm$ and the gas density varies in such a way that the desired modified Knudsen number is achieved in the center of the channel. The exact value of the number of the argon atoms, n_{ssc} , n_{ave} and the gas density in the center of the channel for each case are presented in their corresponding tables. It should be noted that in order to avoid the figures to become confusing, the temperature and density profiles are shown for some selected values in the remainder of the manuscript.

Fig. 1. Perspective and side view of the simulation domain for $k = 10$.

Table 1
MD simulation parameters for $100\epsilon\sigma^{-2} < K_S < 1000\epsilon\sigma^{-2}$.

k	n_{SSC}	n_{AVE}	# atoms	$\rho_{bulk}(\text{kg/m}^3)$	$k_C(\text{mW/mK})$
10	20×10^6	100×10^6	450	1.8	17.85
1	5×10^6	30×10^6	4500	18	18.3

3. Results and discussion

In the first set of simulations, the wall mass and wall/gas interaction strength are set to $m_{wall} = m_{Ar}$ and $\epsilon_{wall-Ar} = \epsilon_{Ar-Ar}$, while the wall spring stiffness value changes as $100\epsilon\sigma^{-2} < K_S < 1000\epsilon\sigma^{-2}$. The simulation parameters are summarized in Table 1.

Fig. 2. Distribution of argon gas density along the channel height (a and b), near the top (c and d) and the bottom wall (e and f) for different K_S .

The density distributions of argon gas along the channel height and within $2nm$ from the cold and the hot walls for different wall spring stiffness in the range of $100\epsilon\sigma^{-2}$ to $1000\epsilon\sigma^{-2}$ are depicted in Fig. 2. It is shown that the variation of wall stiffness does not notably change the argon gas distribution along the channel height therefore, ρ_{bulk} does not change notably as K_s varies for each Knudsen number. The only difference can be observed in the wall force field region and for $K_s = 150\epsilon\sigma^{-2}$, where a reduction in the maximum gas density near the walls is observed.

Fig. 2 depicts that the maximum argon gas density near the cold walls are 6.25kg/m^3 and 61.45kg/m^3 for $k = 10$ and $k = 1$, respectively. As the wall stiffness reduces to $150\epsilon\sigma^{-2}$, these values are reduced to 5.71kg/m^3 and 56.4kg/m^3 . The same phenomena are observed near the hot wall. These reductions are in full accordance with the distribution of liquid molecules near the solid walls as the wall stiffness varies [60]. For small values of the wall stiffness, e.g. $150\epsilon\sigma^{-2}$, the wall molecules oscillate with higher amplitudes around their equilibrium position which enables them to penetrate

Fig. 3. Distribution of argon gas temperature along the channel height (a and b), near the top (c and d) and the bottom wall (e and f) for different K_s .

Fig. 4. Heat flux and effective thermal conductivity as a function of K_s for $k = 10$ and 1.

farther into the adjacent gas medium. Increased penetration of the wall molecules through the gas medium prevents the gas atoms to get too close to the wall structure. As the wall stiffness increases, the solid atoms oscillation amplitude reduces so the gas atoms can get closer to the walls and forms a stronger density peak. Fig. 2 shows that the variation of the maximum gas density near each wall as a function of wall stiffness has the same trend as the liquid-solid medium.

It is worth mentioning that the gas density distribution is not symmetric along the channel width as shown in Fig. 2. Different temperatures, 308K and 288K, were assigned to the top and the bottom wall, respectively, so the gas temperature is between those two limiting conditions. Since the top wall is a hotter than the gas, the wall molecules oscillate with higher energy in comparison with the gas atoms. As the gas atoms hit the wall, they absorb energy

from the wall so they can escape from the wall force field region with higher velocity. This results in a reduction of the gas atom density near the top wall. In contrast, as the gas atoms hit the cold bottom wall, they loose energy and transfer it to the wall molecules. Thus, their residence time near the wall region is higher and the density distribution of gas atoms near the bottom wall increases. Since the temperature difference between the walls is 20K, the difference between the density peaks near the hot and cold walls is small [48]. As an example in Fig. 2c and 2e, the maximum density for $K_s = 150\epsilon\sigma^{-2}$ near the hot and cold walls are 5.08kg/m³ and 5.71kg/m³, respectively. Similarly, for $K_s = 900\epsilon\sigma^{-2}$, these density peaks become 5.84kg/m³ and 6.24kg/m³ for the hot and cold walls, respectively. It should be considered that as the temperature difference increases, the difference between the density peaks increases [46,49].

Fig. 3 shows the variation of the temperature profile along the channel height and within 2nm from the cold and the hot walls. Fig. 3a and 3b depict the distribution of the gas temperature along with the channel height as the wall spring stiffness varies between $100\epsilon\sigma^{-2}$ to $1000\epsilon\sigma^{-2}$ for $k = 10$ and $k = 1$, respectively. It is inferred from these figures that regardless of the Knudsen number, the temperature distribution in the bulk region of the gas domain is approximately independent of the wall stiffness. On the other hand, in the wall force field region the wall stiffness becomes a determining factor in the distribution of the temperature within the gas. According to Fig. 3e, near the cold wall and for $k = 10$, the temperature jump is about 4 °C and 6 °C for $150\epsilon\sigma^{-2}$ and $900\epsilon\sigma^{-2}$ wall stiffness, respectively. It is obvious that increasing the wall stiffness leads to a higher temperature jump in the wall force field region. The same trend is observed for $k = 1$ in Fig. 3f and even near the hot walls for both Knudsen numbers in Fig. 3c and 3d. It is known that the temperature jump at the fluid/solid boundary is caused by the difference between the thermal velocity distribution in the fluid and the adjacent wall particles [47]. As the wall stiffness increases, the strong restoring forces acting on the solid particles dampen the effects of the collisions of the gas atoms [50]. Therefore, the difference between the thermal velocity of the

Table 2
MD simulation parameters for $0.5 \leq m_{\text{wall}}/m_{\text{Ar}} \leq 6$.

k	n_{ssc}	n_{ave}	# atoms	$\rho_{\text{bulk}}(\text{kg/m}^3)$	$k_c(\text{mW/mK})$
10	20×10^6	100×10^6	450	1.8	17.85
1	5×10^6	30×10^6	4500	18	18.3

Fig. 5. Density distribution of argon gas along the channel height for different. $m_{\text{wall}}/m_{\text{Ar}}$.

wall and the colliding gas atoms at the interface increases notably which leads to higher temperature jump.

This can also be observed in Fig. 4 which shows the reduction of the heat flux as the wall spring constant increases regardless of the Knudsen number. Fig. 4 depicts that for $k = 10$, as the wall stiffness increases from $150\epsilon\sigma^{-2}$ to $900\epsilon\sigma^{-2}$, the corresponding heat flux reduces from 1.1MW/m^2 to 0.51MW/m^2 . This considerable reduction (about 50%) is referred to the decrement in the energy transfer between the gas and the solid wall atoms as the wall stiffness

increases. The same trend is also observed for a modified Knudsen number of 1, which means the effect of the gas density on the general trend is negligible. Considering the Knudsen number in our study, it is known that Fourier's law is not valid anymore and we have to use the "effective thermal conductivity" concept as $K_{\text{eff}} = J\Delta T/H$ [68] instead, as shown in Fig. 4.

Besides, it should be noted that there is a small kink in the temperature profile near each wall in $0.2\text{nm} < y < 0.4\text{nm}$ which can be named as the near-wall layer. The reduction in gas temperature in

Fig. 6. Distribution of argon gas temperature along the channel height (a and b), near the top (c and d) and the bottom wall (e and f) for different. $m_{\text{wall}}/m_{\text{Ar}}$.

Fig. 7. Heat flux and effective thermal conductivity as a function of $m_{\text{wall}}/m_{\text{Ar}}$ for $k = 10$ and 1.

the near-wall layer occurs due to the strong repulsive force between the wall/gas atoms in the adjacent vicinity of the walls [46,48,49]. Fig. 2 depicts that the gas density reduces notably due to the presence of the repulsive force in the near-wall layer, in comparison with the density-peak at $y = 0.4 \text{ nm}$. Considering that the gas temperature evolved through the gas/gas and the gas/wall atom collisions, the rate of collisions in each layer determines how close to the wall temperature the gas layer temperature can become. Due to the lower density, the gas atoms in the near-wall layer experience lesser gas/gas and gas/wall collisions as compared to the gas atoms in the density-peak layer. Therefore, the gas atoms in the near-wall layer are at a lower temperature in comparison with the gas atoms in the density-peak layer which have the closest temperature to the wall temperature.

In the second set of simulations, the wall stiffness and wall/gas interaction strength are considered as $K_S = 500 \text{ eV} \cdot \text{\AA}^{-2}$ and $\epsilon_{\text{wall-Ar}} = \epsilon_{\text{Ar-Ar}}$ while the wall mass changes as $0.5 \leq m_{\text{wall}}/m_{\text{Ar}} \leq 6$. The simulation parameters are summarized in Table 2. It can be observed that ρ_{bulk} does not change notably as $m_{\text{wall}}/m_{\text{Ar}}$ varies for each Knudsen number. The density distribution of the argon gas along the channel height and within 2 nm from the cold and the hot walls are depicted in Fig. 5. It is shown that the variation of wall mass does not change the argon gas distribution along the channel height considerably. The reason for this behavior refers to the fact that the oscillation amplitude of the wall atoms is a function of wall temperature and that the mass of the wall atoms has a negligible effect. This is consistent with previous observations for liquid/solid interactions [60,61]. Fig. 6 depicts the varia-

tion of the temperature profile along the channel height and in a distance of 2 nm from the cold and the hot walls as a function of wall atom mass. It is shown that regardless of the Knudsen number, the maximum temperature jump is observed for $m_{\text{wall}}/m_{\text{Ar}} = 0.5$ near the hot and cold walls. It is observed that as $m_{\text{wall}}/m_{\text{Ar}}$ increases to 2, the temperature jump reduces which means that the momentum and heat transfer between the gas and the walls enhances notably. According to Fig. 6, a further increase in the ratio of $m_{\text{wall}}/m_{\text{Ar}}$ up to 6 results in an increase of the corresponding temperature jump. As an example, the temperature jump near the cold wall for $k = 10$ is about 6.14, 4.4 and 5 K if the ratio of $m_{\text{wall}}/m_{\text{Ar}}$ is assumed to be equal to 0.5, 2 and 6, respectively. The same trend is also observed for $k = 1$ and even near the hot walls.

The reduction and increment of the temperature jump as the ratio $m_{\text{wall}}/m_{\text{Ar}}$ changes from 0.5 to 6 is referred to the combination of two opposite phenomena. On the one hand, it is observed that for liquid/solid interactions, as the mass of the wall atoms increases, the slip length reduces notably which corresponds to a higher momentum transfer between the wall and the fluid atoms [60] as the fluid atoms hit the heavier wall particle. On the other hand, increasing the mass of the wall atoms for constant wall stiffness (as it is the case here) notably reduces the oscillation frequency of the wall atoms. Therefore, it is expected that a reduction happens in the collision rate between the gas and the wall atoms, which leads to an incomplete energy and momentum transfer between them. The combination of these two counteracting phenomena leads to the fact that the most efficient collision (minimum temperature jump) between the gas and wall atoms happens for $m_{\text{wall}}/m_{\text{Ar}}$ about 2. As the ratio $m_{\text{wall}}/m_{\text{Ar}}$ changes from 0.5 to 2, the wall atoms become heavier which leads to a higher momentum and energy transfer between the wall and the impinging gas atoms. This is clearly observed in Fig. 7 which shows the variation of heat flux and thermal conductivity as $m_{\text{wall}}/m_{\text{Ar}}$ changes. It is shown that for $k = 10$, as $m_{\text{wall}}/m_{\text{Ar}}$ increases from 0.5 to 2, the heat flux increases from 0.29 MW/m^2 to 1.04 MW/m^2 . The same trend is also observed for $k = 1$. Higher heat flux reduces the corresponding temperature jump at the interface considerably. As $m_{\text{wall}}/m_{\text{Ar}}$ changes from 2 to 6, the reduction of the oscillation frequency of the wall atoms and consequently reduction of the gas-wall collisions become the dominant factor. This results in a reduction of energy transfer between the wall and the gas which means a higher temperature jump. This is clearly observed in Fig. 7 which shows that for $k = 10$, an increment in $m_{\text{wall}}/m_{\text{Ar}}$ up to 6 reduces the heat flux to 0.58 MW/m^2 . The corresponding effective thermal conductivity is also shown in Fig. 7.

In the third set of simulations, the wall stiffness and the wall mass are considered as $K_S = 500 \text{ eV} \cdot \text{\AA}^{-2}$ and $m_{\text{wall}} = m_{\text{Ar}}$, while the wall/gas interaction strength changes as $1 \leq \epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}} \leq 6$. The simulation parameters for this set of simulations are summarized in Table 3. Due to the variation in wall/gas interaction

Table 3
MD simulation parameters for $1 \leq \epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}} \leq 6$.

k	$\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$	n_{ssc}	n_{ave}	# atoms	$\rho_{\text{bulk}} (\text{kg/m}^3)$	$k_c (\text{mW/mK})$
10	1	20×10^6	100×10^6	460	1.85	17.85
	2			690	1.84	
	3			1570	1.84	
	4			5300	1.86	
	5			16700	1.85	
	6			31500	1.89	
1	1	5×10^6	30×10^6	4600	18.7	18.3
	2			6900	18.8	
	3			13300	18.5	
	4			26500	18.6	
	5			38000	18.8	
	6			44000	18.8	

strength, a different amount of argon gas is adsorbed on the walls. Therefore, in order to keep a constant modified Knudsen number of 1 and 10 in the center of the channel, the number of argon gas atoms varies in such a way that the desired gas density is achieved in the center of the channel by the trial and error method. The density distribution of argon gas along the channel height and within 2nm from the cold and the hot walls is depicted in Fig. 8. Considering the wall force field region near the cold wall $k = 10$, it is observed that the maximum gas density is about 6.2 as $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ equals to 1. As this ratio increases up to 4, the overall

trend of the gas density distribution is the same and all curves show only one single peak.

As $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ varies from 4 to 6, it is observed that a second peak is formed in the wall force region which is much weaker than the first one. The maximum gas density near the first peak is about 3892 kg/m^3 while near the second peak, it is reduced to 11.97 kg/m^3 . Considering $k = 1$, the same trend is also observed. For $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ being equal to 1, the gas density distribution experiences a single peak at about 61.35 kg/m^3 . Fig. 8f clearly depicts that as this ratio is increased to up to 4, the second peak starts to

Fig. 8. Distribution of argon gas density along the channel height (a and b), near the top (c and d) and the bottom wall (e and f) for different $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$.

form. For $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ equal to 6, the second peak is formed clearly and while the maximum gas density near the first peak is around 4500kg/m^3 , for the second peak it reaches to 127kg/m^3 . Comparing $k = 10$ and 1 for $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ equal to 6, it is observed that while the value of the first peaks is of the same order of magnitude, the second peak is much stronger (almost ten times) for $k = 1$. It is interesting to note that regardless of the temperature of the walls and the Knudsen number, the first and second peaks occur at 0.1nm and 0.4nm distance from the walls, respectively.

Fig. 9 shows the variation of the temperature profile along the channel height as a function of the wall/gas interaction strength. It is observed that as the value of $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ increases, the gas-wall interactions become stronger leading to an improved momentum and energy transfer across the gas-solid interface and subsequently to a reduction of the temperature jump. Fig. 9 depicts that regardless of the Knudsen number and the wall temperature, the gas experiences the wall temperature for $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}} \geq 4$.

The increased number of gas atoms at the walls causes a higher collision rate between the gas and the wall atoms which leads to an enhancement of the heat transfer. Fig. 10 clearly shows that for $k = 10$, as $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ increases from 1 to 4 the heat flux varies from 0.76MW/m^2 to 1.46MW/m^2 while further increment up to 6 changes the resulting heat flux to 1.56MW/m^2 . Meanwhile, for $k = 1$, as this ratio changes from 1 to 4, the heat flux varies from 6.83MW/m^2 to 12.37MW/m^2 and further increment up to 6 changes the resulting heat flux to 12.51MW/m^2 . This implies that regardless of the Knudsen number, the induced heat flux between the walls is a function of the gas/wall collision rate and remains almost constant as $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ exceeds 4.

Figs. 4, 7 and 10 show the effect of the wall stiffness, wall mass, and wall interaction strength on the induced heat flux through the gas medium. In this part, we assume different kind of the metals as the wall and use the above-mentioned figures to compare the ability of each material to transfer heat through the gas medium. Silver (Ag), Copper (Cu), Aluminum (Al), Gold (Au), Lead (Pb) and Nickel (Ni) are considered as the wall and their corresponding K_S , $m_{\text{wall}}/m_{\text{Ar}}$ and $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ is determined. Then they have been plotted in Fig. 11, which enables us to approximately compare the induced heat flux in the gas domain for each material. While the metal atom mass and interaction strength have been taken from the previously published data [69], the interaction between the metal and argon is calculated by the well-known Lorentz-Berthelot mixing rule as follows:

$$\epsilon_{ij} = \sqrt{\epsilon_{ii}\epsilon_{jj}} \quad (5)$$

Fig. 10. Heat flux and effective thermal conductivity as a function of $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ for $k = 10$ and 1 .

All the metal walls are built according to the Einstein model, which implies that the wall atoms are attached to the Face-Centered-Cubic (FCC) lattice (110) and oscillate by a harmonic spring. The spring constant in this model is determined as follows [70,71]:

$$K_S = \frac{m_{\text{wall}} K_B^2 T_E^2}{h^2}, \quad (6)$$

in which T_E is the Einstein temperature, m_{wall} is the wall atom mass and h is the reduced Planck constant. It should be noted that the Einstein temperature is computed from the Debye temperature of the metals [72,73], which is usually given for two distinct conditions, the low-temperature limit at 0K and room temperature at 298K . Since in all MD simulations in the present work, 308K and 288K were assigned to the top and the bottom wall, respectively, we have chosen the Debye temperature of the room condition for the metals. The physical and calculated properties of the metals can be found in Table 4.

Using Eq. (6), the calculated K_S is written in the form of $\beta\epsilon\sigma^{-2}$ and β is determined for each metal. Then, they are plotted in Fig. 11(a) and (b) for $k = 10$ and $k = 1$, respectively. Interestingly, it is observed that the resulting wall stiffness does not vary too

Fig. 9. Temperature distribution of argon gas along the channel height for different $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$.

Fig. 11. Induced heat flux through the gas medium for different metals as a function of K_s (a and b), m_{wall}/m_{Ar} (c and d) and $\epsilon_{wall-Ar}/\epsilon_{Ar-Ar}$ (e and f).

much for different metals which is related to their similar FCC structure. Therefore, the resulting heat flux does not vary considerably for these metals which is clearly shown in Fig. 11. In terms of the wall stiffness, while Pb and Ni induced the highest heat flux in the gas medium, Ag induces the least. Fig. 11(c) and (d) depict the variation of induced heat flux as the wall for different metals in our study. It is shown that Ag, Cu, and Ni induce the most heat flux while Al is the least one if the ratio of the wall/gas atoms mass is considered. It is obvious that the difference between the highest

and least induced heat flux is more profound in comparison with changing of the wall stiffness. Finally, the variation of induced heat flux as a function of interaction potential strength is shown in Fig. 11(e) and (f). It is observed that while the least induced heat flux is found for Pb, the other metals induce approximately the same amount of heat flux through the gas medium. Considering these three parameters simultaneously, it seems that Ni, Ag, and Cu enhance the heat transfer through the gas medium in comparison with Au, Pb, and Al. However, it should be noted that what

Table 4
Physical and calculated properties of the metals.

	$T_E(K)$	$\sigma(\text{nm})$	$\epsilon_{\text{metal-metal}}(J)$	$\epsilon_{\text{metal-argon}}(J)$	$\frac{\epsilon_{\text{wall-Ar}}}{\epsilon_{\text{Ar-Ar}}}$	K_S	β	$\frac{m_{\text{wall}}}{m_{\text{Ar}}}$
Ag	172	0.2955	3.17×10^{-20}	0.725×10^{-20}	4.37	90	248	2.7
Cu	248	0.2616	3.28×10^{-20}	0.737×10^{-20}	4.44	110.5	230	1.58
Al	317	0.293	2.79×10^{-20}	0.68×10^{-20}	4.1	77	236	0.68
Au	131	0.295	3.67×10^{-20}	0.78×10^{-20}	4.7	96.06	228	4.93
Pb	76	0.3565	2.04×10^{-20}	0.58×10^{-20}	3.49	34	212	5.19
Ni	276	0.255	3.93×10^{-20}	0.81×10^{-20}	4.86	127	210	1.47

actually determines the induced heat transfer is the combined effect of wall stiffness, wall atom mass and wall interaction strength. It is important to note that the final combination might not have a linear relationship between these three parameters. Therefore, considering the real materials as the walls is still the most accurate way to calculate the induced heat flux through the nanoconfined gas medium. Figs. 4, 7, 10 and 11 depict the overall trend of the induced heat flux variation and can be used to compare different materials as discussed above. Besides, it should be considered that as stated before, the top and bottom walls are at 308K and 288K, respectively and consequently, the gas mean temperature is around 298K. As the temperature difference between the walls increases, the atom distribution along the channel height varies considerably which changes the induced heat flux [49].

4. Conclusion

Three-dimensional molecular dynamics simulations of a stationary argon gas confined in a nanochannel are used to investigate the combined effects of the wall characteristics and the wall force field region in the gas medium on the heat transfer characteristics and gas atom distribution along the channel height. The bottom wall (cold wall) is kept at 288K and the top wall (hot wall) temperature is fixed at 308K. The channel height is 5.4nm and the gas density varies in such a way that the modified Knudsen number in the center of the channel becomes 10 and 1. Considering the fact that approximately 40% of the channel height is affected by the wall force field, it is observed that the heat transfer characteristics of the gas medium and the distribution of the gas atoms along the channel height strongly depend on an interplay between the wall force field, the wall atom mass, the wall stiffness, and the wall/gas potential interaction strength. It is observed that for all cases, the gas density peak appears at 0.1nm away from each wall. Furthermore, it is shown that as the wall stiffness increases from $100\epsilon\sigma^{-2}$ to $1000\epsilon\sigma^{-2}$ for both Knudsen numbers, the resulting heat flux reduces notably about 50% which causes an increase of the temperature jump at the solid/gas interface. As the wall becomes stiffer, a reduction in the wall atoms oscillation amplitude occurs which reduces the gas-wall atoms collision rate and consequently the heat transfer. Besides, it is depicted that the gas density distribution in the bulk region of the channel is almost unaffected from the wall stiffness while the maximum value of that gas density near each wall is lowest for $150\epsilon\sigma^{-2}$ and remains almost constant for higher values of the wall stiffness. In addition, it is observed that the gas atom distribution along the channel height is approximately unaffected as the ratio $m_{\text{wall}}/m_{\text{Ar}}$ increases from 0.5 to 6 while the heat flux increases as $m_{\text{wall}}/m_{\text{Ar}}$ increases from 0.5 to 2 and a reduction occurs as it changes from 2 to 6. Regarding the heat flux, it is observed that the minimum and maximum temperature jump at the interface occurs for $m_{\text{wall}}/m_{\text{Ar}}$ equal to 2 and 0.5, respectively. Actually, as the mass of the wall atoms increases, the combined effect of the increment in energy transfer due to having a higher effective collision and a reduction in the gas/wall number

of collisions as the collision frequency declines, determines the heat transfer characteristics. Moreover, it is observed that as $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ increases above 4, the gas density distribution along the channel height experiences another peak at 0.4nm distance from the walls which is much weaker than the first one. In addition, it is observed that by increasing $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ from 1 to 4, the heat flux through the gas domain is drastically enhanced which leads to a smaller temperature jump at the interface. As the wall/gas interaction increases, the accumulation of the gas atoms in the adjacent layer of the wall increases notably which leads to an increment in gas/wall collisions and consequently the heat transfer. It is observed that a further increase of $\epsilon_{\text{wall-Ar}}/\epsilon_{\text{Ar-Ar}}$ does not change the resulting heat flux notably while there is no temperature jump on the solid/gas interface anymore and the gas experiences the wall temperature. This refers to the fact that a higher increase in the wall/gas interactions does not change the gas atom distribution in the adjacent layer of the wall anymore.

Declaration of Competing Interest

The authors declared that there is no conflict of interest.

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